Dynamics of DNA breathing in the Peyrard-Bishop model with damping and external force

A. Sulaiman[1a], F.P Zen[2b,c], H. Alatas[3d,c], L.T. Handoko[4e,f]

[a]*Badan Pengkajian dan Penerapan Teknologi, BPPT Bld. II (19th floor), Jl. M.H. Thamrin 8, Jakarta 10340, Indonesia*
[b]*Theoretical High Energy Physics and Instrumentation (THEPI), Department of Physics, Institut Teknologi Bandung, Jl. Ganesha 10, Bandung 40132, Indonesia*
[c]*Indonesia Center for Theoretical and Mathematical Physics (ICTMP), Department of Physics, Institut Teknologi Bandung Jl. Ganesha 10, Bandung 40132, Indonesia*
[d]*Theoretical Physics Division, Department of Physics, Bogor Agricultural University, Kampus IPB Darmaga, Bogor,16680 Indonesia*
[e]*Group for Theoretical and Computational Physics, Research Center for Physics, Indonesian Institute of Sciences, Kompleks Puspiptek Serpong, Tangerang 15310, Indonesia*
[f]*Department of Physics, University of Indonesia, Kampus UI Depok, Depok 16424, Indonesia*

Abstract

The impact of damping effect and external forces to the DNA breathing is investigated within the Peyrard-Bishop model. In in the continuum limit, the dynamics of the breathing of DNA is described by the forced-damped nonlinear Schrodinger equation and studied by means of variational method. The analytical solutions are obtained for special cases. It is shown that the breather propagation is decelerated in the presence of damping factor without the external force, while the envelope velocity and the amplitude increase significantly with the presence of external force. It is particularly found that the higher harmonic terms are enhanced when the periodic force is applied. It is finally argued that the external force accelerates the DNA breathing.

Keywords: DNA-breathing; Peyrard-Bishop; soliton

[1]Email : albertus.sulaiman@bppt.go.id
[2]Email : fpzen@fisika.itb.ac.id
[3]Email : alatas@ipb.ac.id
[4]Email : handoko@teori.fisika.lipi.go.id, laksana.tri.handoko@lipi.go.id

1. Introduction

It is well known that the biological molecule functions such as transcription and replication can not be explained only by their static structure but also by their dynamical behavior [1]. The transcription processes begun with separation of the double helix into a single helix called denaturation process [2]. The famous model for explaining thermal denaturation is the Peyrard-Bishop (PB) model [3]. The model consists of two chains connected by Morse potential representing the hydrogen (H) bonds. It has been shown that the H bonds stretching depends on the coupling constant and temperature, while in the continuum limit satisfies the Nonlinear Schrodinger equation. The solution of Nonlinear Schrodinger equation is implies for a self-focusing case could initiate the denaturation [3]. The intensive studies on PB model have been done for example, the molecular dynamics calculation [4], including anharmonics nearest-neighbor stacking interaction [5], connection with conformation of local denaturation[6], the effects of stacking interactions [7] and the Monte-Carlo simulation [8].

Even under physiological conditions, the DNA double-helix spontaneously denatures locally, opening up and fluctuating, and have a large amplitude localized excitations called DNA breathing [9, 10]. It is well known that the thermal denaturation of double strands DNA depend on the solution that surrounding the DNA molecules [11]. Using this fact, it is necessary to take into consideration that the solving water does act as a viscous medium that could damp out DNA breathing. The impact of viscosity was investigated by Zdrakovic et al [12]. The behavior of DNA dynamics in viscous solution is described by the damped nonlinear Schrodinger equation. In the other hand, the experiment showed that the double stranded DNA can be separated by applying a fixed external force [13]. It was shown that the observed phase diagram for the unzipping of double stranded DNA is much richer than the earlier suggestion theoretical work. Therefore, it is necessary to improve the PB model to take into account a viscosity and the external forced simultaneously. To our knowledge, this problem has never been reported elsewhere.

This paper discusses the viscous dissipation effect as well as an external force acting to DNA in the Peyrard-Bishop models. In the section (2) formulation of the impact of a damping and external force is derived. The

continuum approximation to describe DNA breathing is described in section (3). Soliton solution based on the variational method is given in section (4). The breathing dynamics in term of solitary waves is discussed in section (5). The paper is ended with a summary.

2. Peyrard-Bishop Model with damping and external forces

Following the PB model, the motion of DNA molecules is represented by two degree of freedom u_n and v_n which correspond to the displacement of the base pair from their equilibrium position along the direction of the hydrogen bonds connecting the two base in pair in two different strands [3]. Making a transformation to the center of mass coordinate representing the in phase and out of phase transverse motions, $X_n = (u_n + v_n)/\sqrt{2}$ and $Y_n = (u_n - v_n)/\sqrt{2}$ respectively, the Hamiltonian of the PB model is given by [3],

$$
\begin{aligned}
H &= \sum_n \frac{1}{2M}(p_n)^2 + \frac{\kappa}{2}(X_{n+1} - X_n)^2 + \sum_n \frac{1}{2M}(P_n)^2 \\
&\quad + \frac{\kappa}{2}(Y_{n+1} - Y_n)^2 + \frac{D}{2}(e^{-\frac{\alpha}{2}Y_n} - 1)^2 ,
\end{aligned}
\tag{1}
$$

where D and α are the depth and inverse width of the potential respectively. The momentum $p_n = M\dot{X}_n$, $P_n = M\dot{Y}_n$ and κ is the spring constant.

As mentioned above, the studies of PB models that included the viscosity was done by adding the term $-\epsilon\gamma\dot{Y}_n$ in the equation of motion (EOM) [12]. In ref. [12] the nonlinear Schrodinger equation with viscous effect was solved to study the dynamics of DNA breathing. The interaction between the system with it's environment lead dissipation of energy. This means that the system is not longer conservative and reversible. The corresponding Hamiltonian formulation for dissipative system is called Caldirola-Kanai Hamiltonian in the form of a time-dependent Hamiltonian which defined as follow [14],

$$
H = e^{-\gamma t}\frac{p^2}{2m} + e^{\gamma t}V(x) ,
\tag{2}
$$

where $\gamma = \eta/M$, η is damping coefficient. The model has been used to study the quantum dissipation such as the quantization of an electromagnetic field inside a resonator filled by dielectric medium [15], study of susceptibility for identical atoms subjected to an external force [16], coherent states for the damped harmonic oscillator[16], dissipative tunneling of the inverted

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Caldirola-Kanai oscillator [17] and functional integral for non-Lagrangian systems [18].

In principle one can extend their approach to describe the denaturation processes in a dissipation system. We propose that the PB model with the damping effect and an external driving force $F(t)$ is defined as follow,

$$H_x = \sum_n e^{-\gamma t} \frac{p_n^2}{2m} + e^{\gamma t} \frac{\kappa}{2} (X_{n+1} - X_n)^2 + e^{\gamma t} F_n(t) X_n , \qquad (3)$$

$$H_y = \sum_n \frac{e^{-\gamma t}}{2M} (P_n)^2 + \frac{e^{\gamma t} \kappa}{2} (Y_{n+1} - Y_n)^2$$

$$+ \frac{e^{\gamma t} D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1)^2 + e^{\gamma t} F_n(t) Y_n , \qquad (4)$$

Here $F_n(t)$ is a conservative force. Substituting into the Hamilton equation yield,

$$\dot{Y}_n = \frac{\partial H_y}{\partial P_n} = e^{-\gamma t} \frac{P_n}{M}$$

$$\dot{P}_n = -\frac{\partial H_y}{\partial Y_n} = e^{\gamma t} \kappa (Y_{n+1} - 2Y_n + Y_{n-1})$$

$$+ e^{\gamma t} \frac{\alpha D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1) + e^{-\frac{\alpha}{2} Y_n} + e^{\gamma t} F_n(t) . \qquad (5)$$

Next, by substituting first equation into the second equation we find the corresponding EOM as follow,

$$M \ddot{Y}_n + M \gamma \dot{Y}_n = \kappa (Y_{n+1} - 2Y_n + Y_{n-1})$$

$$+ \frac{\alpha D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1) e^{-\frac{\alpha}{2} Y_n} + F_n(t) . \qquad (6)$$

In the mean time, the EOM for X_n satisfies the following damped harmonic oscillator with external forcing,

$$M \ddot{X}_n + M \gamma \dot{X}_n - \kappa (X_{n+1} - 2X_n + X_{n-1}) + F_n(t) = 0 . \qquad (7)$$

The damping term $m \gamma \dot{Y}_n$ is similar with [12], where they add a new force $F_n = -\gamma \dot{Y}_n$ in the EOM.

3. Continuum Limit Approximation

The dynamical behavior of DNA breathing can be studied by applying the continuum approximation on the equation (7). We assume that the amplitude of oscillation is small and the nucleotide oscillate around the bottom of the Morse potential but large enough due to nonlinear effect. We use the following approximation [1, 12, 19],

$$Y_n = \epsilon \Psi_n; (\epsilon \ll 1) . \tag{8}$$

Substituting Eq.(8) into Eq.(6) and retained up to the third order of the Morse potential, we get

$$
\begin{aligned}
\ddot{\Psi}_n \;+\;& \gamma \dot{\Psi} = \omega_0^2 (\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}) \\
\;+\;& C_m^2 (\Psi_n + \epsilon a_1 \Phi_n^2 + \epsilon^2 a_2^2 \Psi_n^3) + \tilde{F}_n ,
\end{aligned}
\tag{9}
$$

where $\omega_0^2 = \frac{\kappa}{M}$, $C_m^2 = \frac{\alpha^2 \bar{D}}{2M}$, $a_1 = -\frac{3}{4}\alpha$, $a_2 = \alpha\sqrt{\frac{7}{24}}$, $\bar{D} = 1/N \sum_n^N D_n$ is the average value of D and $\tilde{F}_n = F_n(\epsilon \Psi_n)$. For a relatively long DNA chain, this equation can be simplified by taking full continuum limit approximation which should be valid as long as the solution under consideration changes rather slowly and smoothly along with DNA [2]. This approximation yields,

$$\frac{\partial^2 \Psi}{\partial t^2} + \gamma \frac{\partial \Psi}{\partial t} = C_0^2 \frac{\partial^2 \Psi}{\partial x^2} + C_m^2 (\Psi + \epsilon a_1 \Phi^2 + \epsilon^2 a_2^2 \Psi^3) + \tilde{F}(x,t) , \tag{10}$$

where $C_0^2 = \omega_0^2 l^2$ and l is a length scale. The term of $\epsilon \tilde{F}(x,t)$ and $\epsilon \gamma \partial \Psi / \partial t$ can be treated as a perturbation by assuming that it contributes small enough to the whole DNA motion which should be dominated by the first and second terms yielding a solution of $\Psi \sim e^{i(kx - \omega t)}$. Then, using the multiple scale expansion method, namely by expanding the associated equation into different scale and time spaces [20],

$$
\begin{aligned}
\Psi \;&=\; \Psi^{(0)} + \epsilon \Psi^{(1)} + \cdots , &\tag{11} \\
\frac{\partial}{\partial t} \;&=\; \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \cdots , &\tag{12} \\
\frac{\partial}{\partial x} \;&=\; \frac{\partial}{\partial x_0} + \epsilon \frac{\partial}{\partial x_1} + \cdots . &\tag{13}
\end{aligned}
$$

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and by substituting this expansion into Eq. (10), one obtains,

$$
\begin{aligned}
0 \quad =\epsilon^0 &\left[\frac{\partial^2 \Psi^{(0)}}{\partial t_0^2} - C_0^2 \frac{\partial^2 \Psi^{(0)}}{\partial x_0^2} - C_m^2 \Psi^{(0)} \right] \\
+\epsilon^1 &\left[\frac{\partial^2 \Psi^{(1)}}{\partial t_0^2} + 2\frac{\partial^2 \Psi^{(0)}}{\partial t_0 \partial t_1} - C_0^2 \frac{\partial^2 \Psi^{(1)}}{\partial x_0^2} + \gamma \frac{\partial \Psi^{(1)}}{\partial t_0} \right. \\
&\left. -2C_0^2 \frac{\partial^2 \Psi^{(0)}}{\partial x_0 \partial x_1} + C_m^2 \Psi^{(1)} - \frac{3}{2} C_m^2 (\Psi^{(0)})^2 + \tilde{F} \right] \\
+\epsilon^2 &\left[\frac{\partial^2 \Psi^{(0)}}{\partial t_1^2} + 2\frac{\partial^2 \Psi^{(1)}}{\partial t_0 \partial t_1} - C_0^2 \frac{\partial^2 \Psi^{(0)}}{\partial x_1^2} \right. \\
&\left. -2C_0^2 \frac{\partial^2 \Psi^{(1)}}{\partial x_0 \partial x_1} + \frac{7}{6} C_m^2 (\Psi^{(0)})^3 + 2C_m^2 \Psi^{(0)} \Psi^{(1)} \right] + \dots .
\end{aligned}
\tag{14}
$$

Since the first and second terms in the leading order (LO) and next to leading order (NLO) terms of Eq.(14) provide the harmonic solutions, while the remaining terms lead to non-harmonic solutions, then it is reasonable to consider,

$$
\Psi^{(0)}(x_1, t_1) = \Psi^{(1)}(x_1, t_1) \, e^{i(kx_0 - \omega_0 t_0)} + cc , \tag{15}
$$
$$
\Psi^{(1)}(x_1, t_1) = \Psi^{(0)}(x_1, t_1) + \Psi^{(2)}(x_1, t_1) \, e^{2i(kx_0 - \omega_0 t_0)} + cc , \tag{16}
$$
$$
\tilde{F} = \tilde{f}(x_1) \, e^{i(kx_0 - \omega_0 t_0)} . \tag{17}
$$

Note that the time dependence on the right hand side of Eq. (17) is introduced temporarily just for the sake of convenience, and there are additional charge conjugate terms in each equation. These lead to the order by order EOM,

$$
\Psi^{(0)} = 3 \left| \Psi^{(1)} \right|^2 , \tag{18}
$$
$$
i\frac{\partial \Psi^{(1)}}{\partial \tau} + \Lambda_1 \frac{\partial^2 \Psi^{(1)}}{\partial \xi^2} + \Lambda_2 \frac{\partial \Psi^1}{\partial \tau} \quad + \Lambda_3 \left| \Psi^{(1)} \right|^2 \Psi^{(1)} = \tilde{f} , \tag{19}
$$
$$
\Psi^{(2)} = \frac{1}{2} \left| \Psi^{(1)} \right|^2 , \tag{20}
$$

where $\Lambda_1 = C_0 \bar{D}/(2C_m^3)$, $\Lambda_2 = \gamma/(2C_m)$, $\Lambda_3 = 2\bar{D}/C_m$, $\tau \equiv t_1 = \epsilon t_0$, $\xi \equiv x_1 - (C_0 k/C_m)t_0$, $x_1 = \epsilon x_0$ and a dispersion relation $\omega_0^2 = \bar{D} + C_0^2 k^2$. The EOM of $\Psi^{(1)}$ is nothing else than the forced-damped nonlinear Schrodinger (FDNLS) equation.

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4. Variational Methods

In this section we discuss the solution of the FDNLS by means of variational methods based on the Lagrangian formulation. It is well know that for the case with $\gamma = 0$ and $\tilde{f} = 0$, the Nonlinear Schrodinger equation admits the following traveling wave solution [2, 12, 19],

$$\Psi^{(1)}(\xi, \tau) = A_0 \operatorname{sech}\left[\frac{1}{L}(\xi - u_e \tau)\right] e^{-i(\tilde{k}\xi - \tilde{\omega}\tau)} , \qquad (21)$$

where,

$$A_0 = \sqrt{\frac{[(u_e^2 - 2u_e u_c)]}{(2\Lambda_1 \Lambda_3)}} \qquad (22)$$

$$L = \frac{\sqrt{2\Lambda_1}}{\sqrt{u_e^2 - 2u_e u_c}} \qquad (23)$$

$$\tilde{k} = \frac{u_e}{2\Lambda_1} \qquad (24)$$

$$\tilde{\omega} = \frac{u_e u_c}{2\Lambda_1} \qquad (25)$$

Here, u_e is the envelope wave velocity and u_c is the carrier wave velocity, satisfying $u_e^2 - 2u_e u_c > 0$. By using Eq.(11), Eq.(15), Eq.(16) we obtain the soliton solution as follow,

$$\Psi(x, t) = 2\Psi^{(1)} \cos(kx - \omega_0 t) + \epsilon |\Psi^{(1)}|^2 [3 + \cos(2(kx - \omega_0 t))] , \qquad (26)$$

where $\Psi^{(1)}$ is described by (21).

Based on the corresponding variational methods to solve the damped-forced nonlinear Schroedinger equation, one can use the solution (21) as the related basic form and considering its amplitude, width, phase velocity and the position of the soliton to be time dependent [20, 21?]. For convenient, let us write the 1-soliton in the following form,

$$\Psi^{(1)}(\xi, \tau) = \eta(\tau)\operatorname{sech}[\eta(\xi + \zeta(\tau))] \exp\left(-i[\theta(\tau)\xi + \phi(\tau)]\right) . \qquad (27)$$

The dynamics of η, θ, ζ and ϕ function can be obtained by using the variational methods. The Lagrangian that satisfy the Euler-Lagrange equation [20],

$$\frac{\partial}{\partial \tau}\left(\frac{\partial l}{\partial \Psi_\tau^{(1)*}}\right) + \frac{\partial}{\partial \xi}\left(\frac{\partial l}{\partial \Psi_\xi^{(1)*}}\right) - \frac{\partial l}{\partial \Psi^{(1)*}} = 0 . \qquad (28)$$

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for the FDNLS is given by,

$$
\begin{aligned}
l &= \frac{i}{2}(\Psi_\tau^{(1)}\Psi^{(1)*} - \Psi_\tau^{(1)*}\Psi^{(1)}) - \Lambda_1 \mid \Psi_\xi^{(1)} \mid^2 +\Lambda_3 \mid \Psi^{(1)} \mid^4 \\
&+ \frac{\Lambda_2}{2}(\Psi_\tau^{(1)}\Psi^{(1)*} - \Psi_\tau^{(1)*}\Psi^{(1)}) - (\tilde{f}\Psi^{(1)*} + \tilde{f}^*\Psi^{(1)}).
\end{aligned}
\tag{29}
$$

Substituting equation (27) into the equation (29) and using $L = \int_{-\infty}^{\infty} l d\xi$, $\int_{-\infty}^{\infty} \mathrm{sech}(a\xi)d\xi = \pi/a$ and $\int_{-\infty}^{\infty} \mathrm{sech}^2(a\xi)\tanh(a\xi)d\xi = 0$ yield,

$$
L = 2\eta\zeta\dot{\theta} + \eta\dot{\phi} + 2i\Lambda_2\eta\zeta\dot{\theta} + i\Lambda_2\eta\dot{\phi} + 4\Lambda_1\eta\theta^2 + \frac{4}{3}\Lambda_3\eta^3 - \eta\bar{F} ,
\tag{30}
$$

where

$$
\bar{F} = \int_{-\infty}^{\infty} \left(\tilde{f}e^{i[\theta(\tau)\xi+\phi(\tau)]} + \tilde{f}^*e^{-i[\theta(\tau)\xi+\phi(\tau)]} \right) \mathrm{sech}[\eta(\xi - \zeta(\tau)]d\xi.
\tag{31}
$$

Eq. (30) is the Lagrange function in term of θ, η, ϕ and ζ. The EOM can be easily obtained by solving the Euler-Lagrange equation,

$$
\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{X}}\right) - \frac{\partial L}{\partial X} = 0 ,
\tag{32}
$$

where $X = (\eta, \theta, \phi, \zeta)$. Substituting the Lagrange function given by Eq.(30) into Eq.(32) leads to the following,

$$
2(1 + i\Lambda_2)\eta\dot{\zeta} + 2(1 + i\Lambda_2)\zeta\dot{\eta} = 8\Lambda_1\eta\theta - \eta\frac{\partial\bar{F}}{\partial\theta}
\tag{33}
$$

$$
2(1 + i\Lambda_2)\zeta\dot{\theta} + (1 + i\Lambda_2)\dot{\phi} = 4(\Lambda_1\theta^2 - \Lambda_3\eta^2) - \eta\frac{\partial\bar{F}}{\partial\eta} - \bar{F}
\tag{34}
$$

$$
(1 + i\Lambda_2)\dot{\eta} = -\eta\frac{\partial\bar{F}}{\partial\phi}
\tag{35}
$$

$$
2(1 + i\Lambda_2)\dot{\theta} = -\frac{\partial\bar{F}}{\partial\zeta}
\tag{36}
$$

Further, by substituting Eq.(35) and Eq.(36) into Eq.(33) and Eq.(34) respectively, we find

$$
(1 + i\Lambda_2)\eta\dot{\zeta} - 4\Lambda_1\theta = 2\eta\frac{\partial\bar{F}}{\partial\eta} - \frac{\partial\bar{F}}{\partial\theta}
\tag{37}
$$

$$
(1 + i\Lambda_2)\dot{\phi} - 4(\Lambda_1\theta^2 - \Lambda_3\eta^2) = \zeta\frac{\partial\bar{F}}{\partial\zeta} - \eta\frac{\partial\bar{F}}{\partial\eta} - \bar{F} .
\tag{38}
$$

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Generally, the analytic solution of the equation (33)-(36) can not be obtained, but it is still possible to find it for special condition. In the next section we restrict ourselves to special case of $\tilde{f}$.

First, let us consider very special case in which the damping factor and external force are vanish ($\Lambda_2 = 0$ and $\bar{F} = 0$). As a result , Eq.(35) show that the function of $\eta = \eta_0$ is a constant and Eq.(36) yield $\theta = \theta_0$ which is also a constant. Eq.(33) and Eq.(34) lead to a simple solutions,

$$\zeta = 4\Lambda_1\theta_0\tau \tag{39}$$
$$\phi = 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)\tau . \tag{40}$$

Such that single soliton have the form of,

$$\Psi^{(1)}(\xi, \tau) = \eta_0\text{sech}\left[\eta_0(\xi + 4\Lambda_1\theta_0\tau)\right] \exp\left(-i[\theta_0\xi + 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)\tau]\right) . \tag{41}$$

Clearly, this is a single soliton solution of the conventional Nonlinear Schrodinger equation.

In the second case, let us ignore the external forces ($\bar{F} = 0$). Again, as a result, Eq.(35) show that the function of $\eta = \eta_0$ is a constant and Eq.(36) yield $\theta = \theta_0$, constant as well. The time dependent variables are ζ that represent of the velocity of soliton and ϕ the phase of soliton. The equation of motion have a simple form as follow,

$$(1 + i\Lambda_2)\frac{d\zeta}{d\tau} - 4\Lambda_1\theta_0 = 0 \tag{42}$$

$$(1 + i\Lambda_2)\frac{d\phi}{d\tau} - 4\left(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2\right) = 0 \tag{43}$$

This yield,

$$\zeta(\tau) = 4\frac{\Lambda_1\theta_0}{(1 + \Lambda_2^2)}\left(1 - i\Lambda_2\right)\tau \tag{44}$$

$$\phi(\tau) = 4\frac{(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)}{(1 + \Lambda_2^2)}\left(1 - i\Lambda_2\right)\tau \tag{45}$$

Finally, the single soliton solution is,

$$\Psi^{(1)}(\xi, \tau) = \eta_0\text{sech}[\eta_0(\xi + \bar{\zeta}\tau) + i\eta_0\bar{\zeta}\Lambda_2\tau]$$
$$\times \exp\left(-\bar{\phi}\Lambda_2\tau\right)\exp\left(-i(\theta_0\xi + \bar{\phi}\tau)\right) , \tag{46}$$

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where $\bar{\zeta} = 4\Lambda_1\theta_0/(1 + \Lambda_2^2)$ and $\bar{\phi} = 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)/(1 + \Lambda_2^2)$.

For the third case, we consider another simple case namely when $\bar{F} = \bar{F}_0$ is a constant. Again we get $\eta = \eta_0$ and $\theta = \theta_0$ are constants. The EOMs in Eq.(37) and Eq.(38) have simple forms as follow,

$$(1 + i\Lambda_2)\frac{d\zeta}{d\tau} - 4\Lambda_1\theta_0 = 0 \tag{47}$$

$$(1 + i\Lambda_2)\frac{d\phi}{d\tau} - 4\left(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2\right) = -\bar{F}_0 \tag{48}$$

This yields,

$$\zeta(\tau) = 4\frac{\Lambda_1\theta_0}{(1 + \Lambda_2^2)}\left(1 - i\Lambda_2\right)\tau \tag{49}$$

$$\phi(\tau) = \left[\frac{4\left(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2\right)}{(1 + \Lambda_2^2)} - \frac{\bar{F}_0}{(1 + \Lambda_2^2)}\right]\left(1 - i\Lambda_2\right)\tau \tag{50}$$

Finally, the single soliton solution for this case is,

$$\begin{aligned}
\Psi^{(1)}(\xi, \tau) &= \eta_0 \exp\left(-\bar{\phi}\Lambda_2\tau\right)\exp\left(F^*\tau\right) \\
&\times \operatorname{sech}[\eta_0(\xi + \bar{\zeta}\tau) + i\eta_0\bar{\zeta}\Lambda_2\tau]\exp\left[-i(\theta_0\xi + \bar{\phi}\tau - F^*\tau)\right]
\end{aligned} \tag{51}$$

where $F^* = \bar{F}_0/(1 + \Lambda_2^2)$. The external force express in the positive exponential term, this show that it will increase the amplitude of the soliton.

In the fourth case, we assume that the amplitude and the phase is a constant $(\eta = \eta_0)$ and $(\theta = \theta_0)$, then the EOM becomes,

$$(1 + i\Lambda_2)\eta_0\dot{\zeta} - 4\Lambda_1\theta_0 = 0 \tag{52}$$

$$(1 + i\Lambda_2)\dot{\phi} - 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2) = \zeta\frac{\partial\bar{F}}{\partial\zeta} - \bar{F}. \tag{53}$$

Further, let us assume that the external force is expressed specifically by

$$\tilde{f} = f_0\exp(-i\theta_0\xi), \tag{54}$$

with f_0 is a constant. Substituting into Eq.(31) yields,

$$\begin{aligned}
\bar{F} &= \int_{-\infty}^{\infty}\left(f_0 e^{-i\theta_0\xi}e^{i[\theta_0\xi + \phi(\tau)]} + f_0 e^{i\theta_0\xi}e^{-i[\theta_0\xi + \phi(\tau)]}\right)\operatorname{sech}[\eta(\xi - \zeta(\tau)]d\xi \\
&= \frac{4f_0}{\pi}\cos(\phi) \tag{55}
\end{aligned}$$

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Such that we find,

$$\dot{\zeta} = \frac{4\Lambda_1\theta_0}{(1+i\Lambda_2)\eta_0} \tag{56}$$

$$\dot{\phi} = -\frac{4f_0}{\pi(1+i\Lambda_2)}\cos(\phi) + \frac{4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)}{(1+i\Lambda_2)} . \tag{57}$$

The Eq.(57) will be solved numerically. It is important to note that the solution of Eq.(57) is a complex function i.e. $\phi = \phi_R + i\phi_I$, such that the soliton profile is given by,

$$\Psi^{(1)}(\xi,\tau) = \eta_0 \exp\left(\phi_I\tau\right)\operatorname{sech}[\eta_0(\xi - \bar{\zeta}\tau) + i\eta_0\bar{\zeta}\Lambda_2\tau]\exp\left[-i(\theta_0\xi + \phi_R\tau)\right] , \tag{58}$$

5. Nonlinear Dynamics of DNA Breathing

The external effects of DNA usually give inhomogeneities in the DNA model. The inhomogeneity in stacking energy is found to modulate the width and speed of the soliton which depend on the nature of the inhomogeneity [?]. The author used the dynamic plane-base rotator model by considering angular rotation of bases in a plane normal to the helical axis. They found that the DNA dynamics is governed by a perturbed sine-Gordon equation. In this paper we found that the inhomogeneities of the DNA breathing dynamics governed by the forced-damped Nonlinear Schrodinger equation. The solutions of the homogeneous case represent a large amplitude with localized oscillatory mode appears as a good explanation of the breathing of DNA and must be spontaneously formed [1, 2, 10].

Let us discuss the previously considered four simple cases. In the first case, it's shown by using transformation $\eta_0 = A_0$ and $\theta_0 = 1/2u_e/\Lambda_1$ that the solution is just the Eq.(21). We simulate the solution for the model parameter given by $\kappa = 8Nm$, $M = 5.1 \times 10^{-25}kg$, $\alpha = 2 \times 10^{10}m^{-1}$, $D = 0.1eV$ and $l = 3.4 \times 10^{-10}m$ is length scale [12]. The system of unit (A^o,eV) defines a time unit $(t.u.)$ equal to $1.021 \times 10^{-14}s$ [22]. The solution demonstrate a sort of a modulated solitonic wave where the hyperbolic and cosine terms correspond to the wave number of the envelope and the carrier wave respectively.

In second case with $\bar{F} = 0$ and damping constant $\gamma = 0.05kg/s$, the behavior of the breathing is depicted in Fig.(1). The figure show that the the breathing propagation along the DNA molecule is effected by the damping.
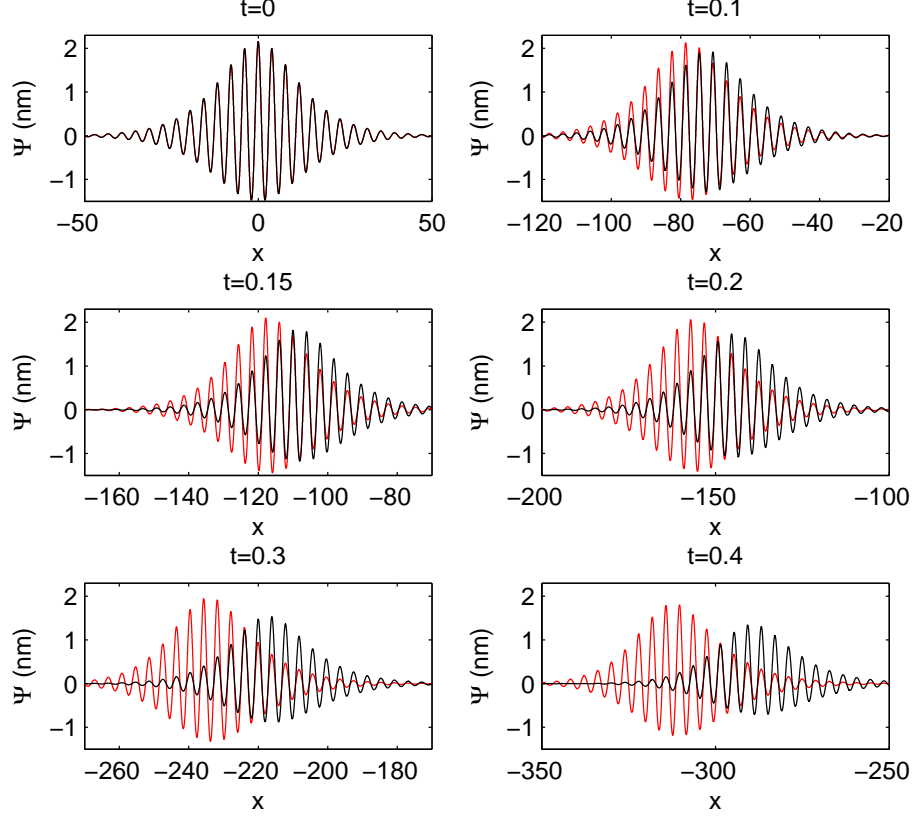
Figure 1: The DNA breathing in the second case where x denotes the continuum base pair in the present model (black) and the original PB model (red) with $g = 0.05$ and $F = 0$.

It is shown from the figure that the damping term decelerates the propagating soliton while retaining its amplitude profile. This indicates that the corresponding damping term does not affects the soliton mass.

Now, consider the solution with the present of the damping effect and $\bar{F} \neq 0$ where the solution is depicted in Fig.(2). The figure is generated with $\bar{F} = 15pN$ and a damping factor $\gamma = 0.05kg/s$. The external force tend to increase the breathing amplitude and damped out by the damping effect. The consequences of this matter, the present of external force tend to increase the envelope velocity significantly. The velocity is increase around $\Delta u_e = \Delta \xi / \Delta \tau \sim 1 order$ in the present of external force $\bar{F} = 15pN$.
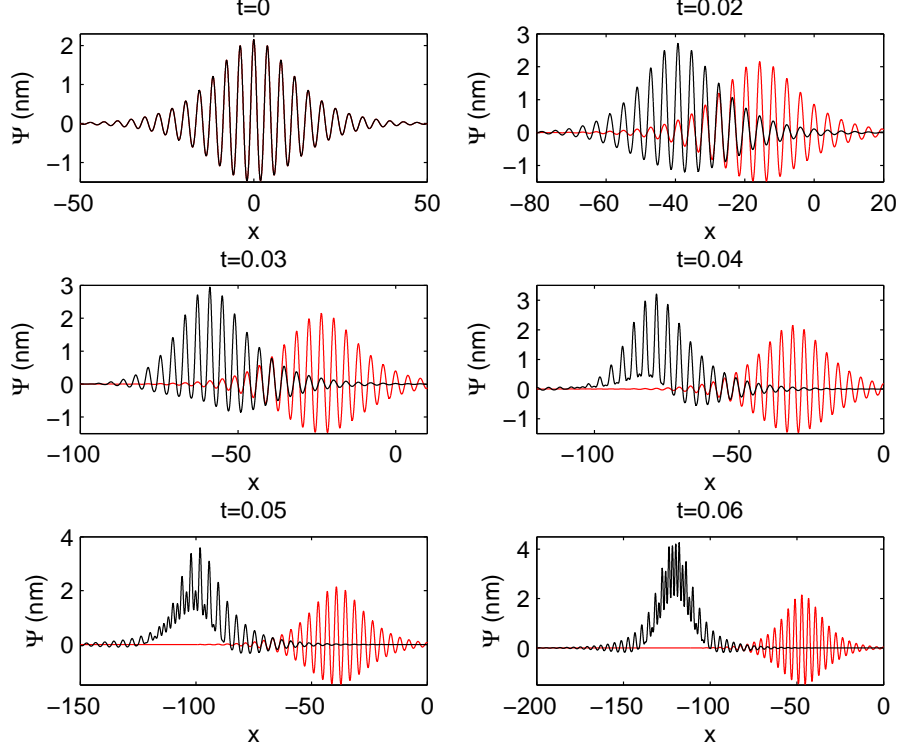
Figure 2: The solitonic solution of DNA breathing in the model with damping effect and external force $\bar{F}$ (black) and in the original PB model (red) with $\gamma = 0.05$ and $\bar{F} = 15$.

Our result is supported by the report given in ref. [23] results. In a cell, DNA strands are separated by the external force [23, 24], or in chemical terms, by enzymes whose interactions with DNA make strands separation thermodynamically favorable at ambient temperature [25]. They showed that the two strands of double-stranded DNA can be separated (unzipped) by the application of $15pN$ force applied at room temperature. Their model predicts that the melting temperature should be a decreasing function of applied force. The paper show that the external force can increase the amplitude of the breathing and may separate the double helix into single helix.

Finally, let us consider the fourth case. The behavior of this case described by on the numerical solution of Eq.(57) which gives a complex function of ϕ. The real part of the solution is associated with the carrier wave, while
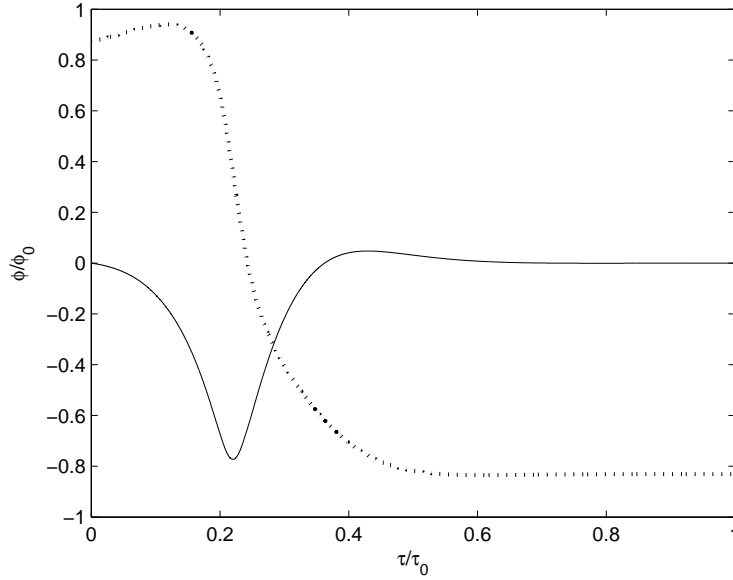
Figure 3: The solution of Eq. (57) where the real and imaginary parts are shown by the dot and solid lines.

the imaginary part with the envelope velocity respectively. The profile of the real part and the imaginary part can be seen in Fig.(3). The real part profile seems to have an anti-sigmoid-like function. In the mean time, the profile of the imaginary part have negative value, which means that the solution propagates to the left direction.

At this point we can consider the solution of FDNLS equation by using Eq.(57) and this is depicted in Fig.(4). Soliton solution of FDNLS show an increasing of the amplitude and its velocity generally tend to increase with time. The amplitude is relatively high and the shape of soliton tend to be step form during it's propagation.

Now, the DNA breathing of the fourth case using the solution of $\Psi^{(1)}$ given in Fig. (4) is depicted in Fig.(5). The amplitude of the DNA breathing is around $2nm$ where the result is similar with ref. [12] for the same parameters. The amplitude of the DNA breathing is relatively increase when its propagate to the left direction. The high amplitude show that the DNA tend to be unzipped and finally completely separate into single helix.

Finally, it is interesting to note the case if we decrease the envelope and carrier velocity respectively in one order. The results is depicted in Fig.(6).
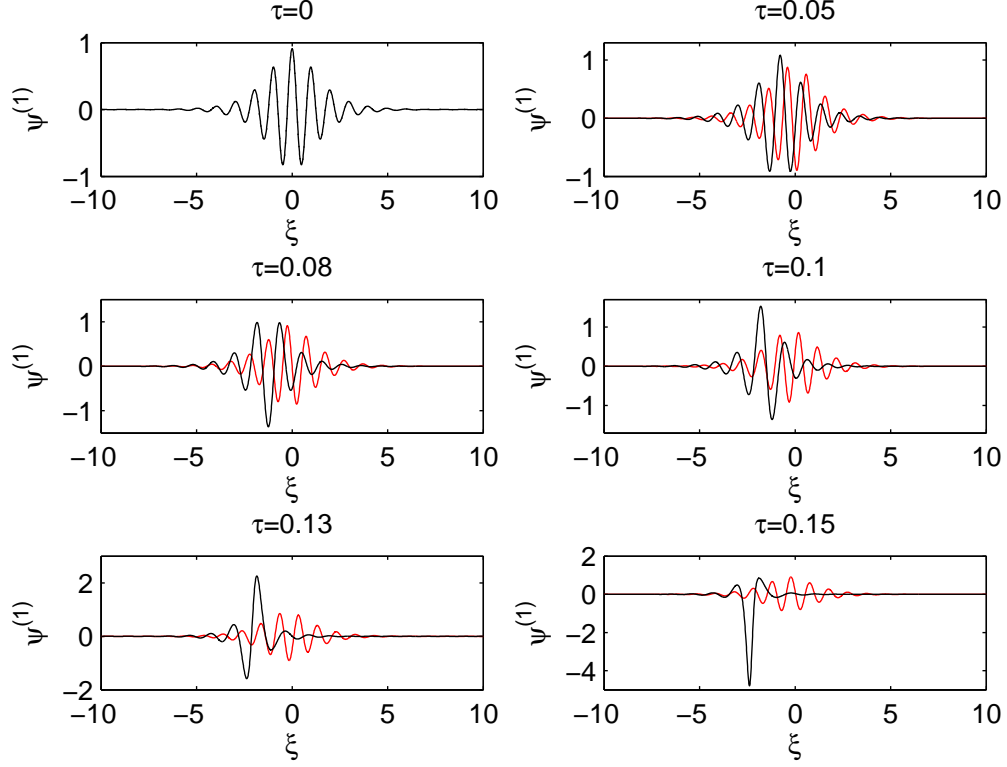
14

Figure 4: The solution of soliton in the FDNLS (black) and the NLS (red) with $\gamma = 0.05$, $\bar{F} = 15\mathrm{e}^{i\xi}$, $v_e = 10^5$ m/s and $u_c = 4 \times 10^4$ m/s.

In this case, the solution of FDNLS propagates more slower than the previous one. At $\tau = 0.3$ the soliton with periodic external force tend to increase its amplitude and velocity. Further at $\tau = 0.6$ the amplitude increase significantly and the corresponding form is change significantly. At $\tau = 0.7$ the higher harmonic term is developed and completely forms at $\tau = 0.9$. As the times goes up the amplitude tend to decrease and disperse into wider form and then the higher harmonic term is generated and increase the amplitude. It is interesting to pointed out that the harmonic term come from the the solution of Eq.(57) that is a nonlinear equation.

The DNA breathing corresponds to the $\Psi^{(1)}$ above is depicted in Fig.(7). The result shows that the amplitude is about $0.2nm$ which is the same with
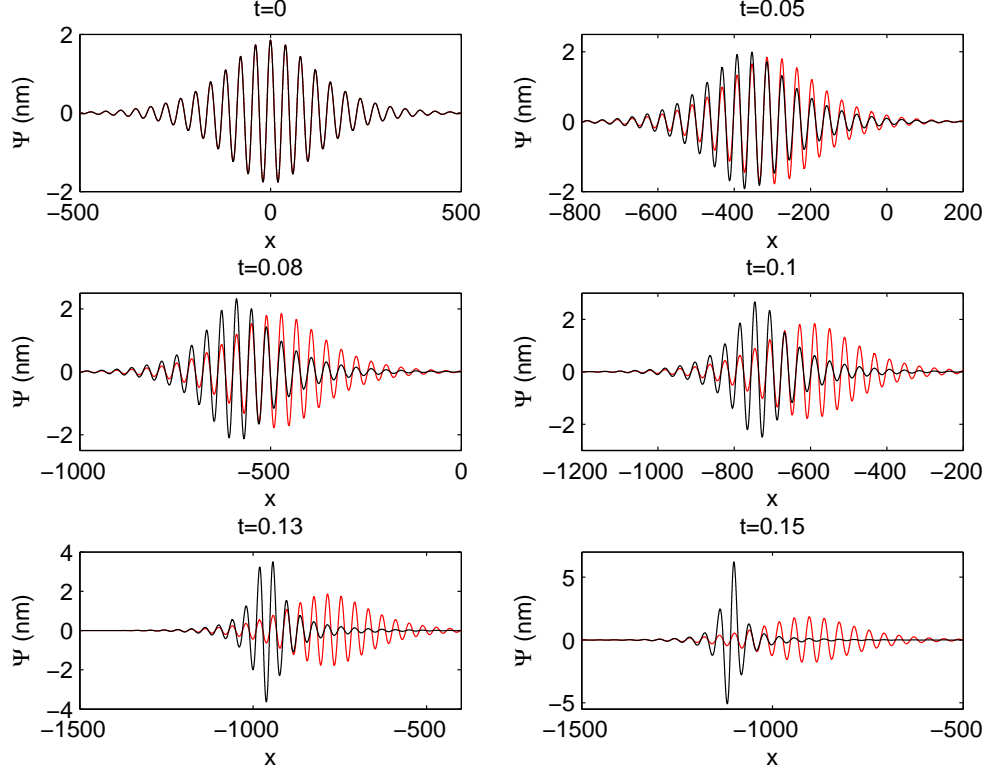
15

Figure 5: The DNA breathing propagation for the fourth case in the present model (black) and the original PB model (red) with $\gamma = 0.05$, $\bar{F} = 15e^{i\xi}$, $v_e = 10^5$ m/s and $u_c = 4 \times 10^4$ m/s.

the result found in ref. [22] in which they used the Forinash-Cretary-Peyrard model with helicosity taken into account. They showed that the opening of the double helix of the DNA itself is controlled by the resonance mode.

As the result shows that the periodic external force and the damping effect generate a higher harmonic term in the dynamics of FDNLS solution then it can be concluded that this phenomenon is responsible for the dynamics of the breathing of the DNA. At this point, we can see that in the early propagation process the DNA breathing tend to decrease its amplitude and disperse into a wider form. The condition changes when the higher harmonic term of FDNLS soliton begin to develop which leads the amplitude of the
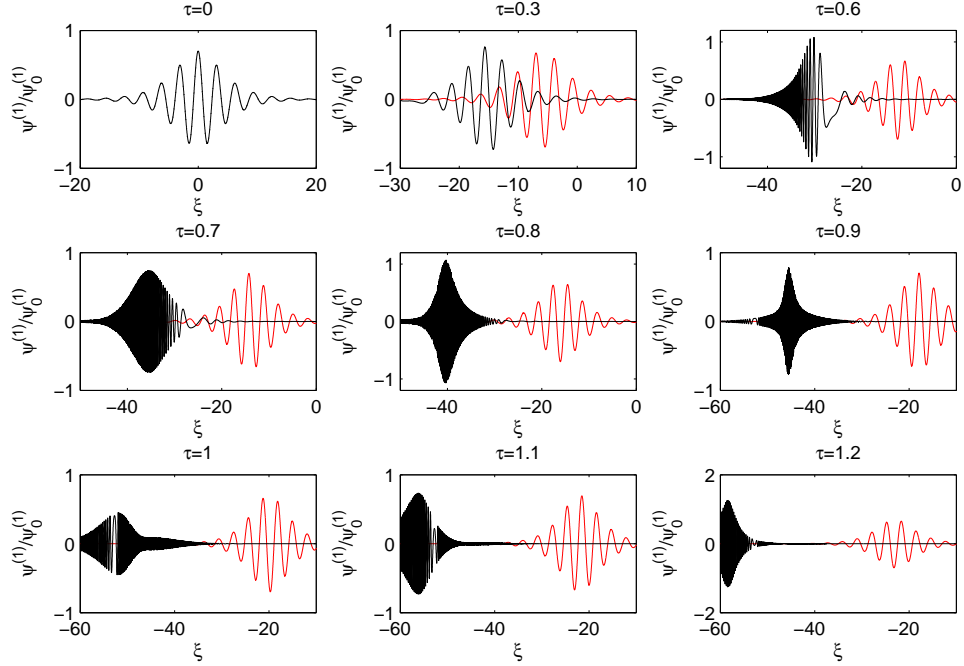
Figure 6: The solution of FDNLS (black) and NLS (red) with $\gamma = 0.05$, $\bar{F} = 15e^{i\xi}$, $K = 4$ Nm, $v_e = 10^4$ m/s and $u_c = 4 \times 10^3$ m/s.

DNA breathing increases significantly.

6. Summary

The impact of viscous fluid and external forces to the Peyrard-Bishop DNA breathing is investigated. We have proposed a PB model with the damping effect and the external driving force which is described by an extended time-dependent Caldirola-Kanai Hamiltonian. Taking full continuum approximation and using the multiple scale expansion method, the EOM is nothing else than the FDNLS equation. Assuming small perturbation of damping and external forces, the FDNLS equation can be solved using the variational methods. The analytical solution have been obtained for only special cases. In the case with damping factor and without external force, the breathing propagation is decelerated by the damping effect. In the presence of external force, the velocity and the amplitude increase significantly. It is
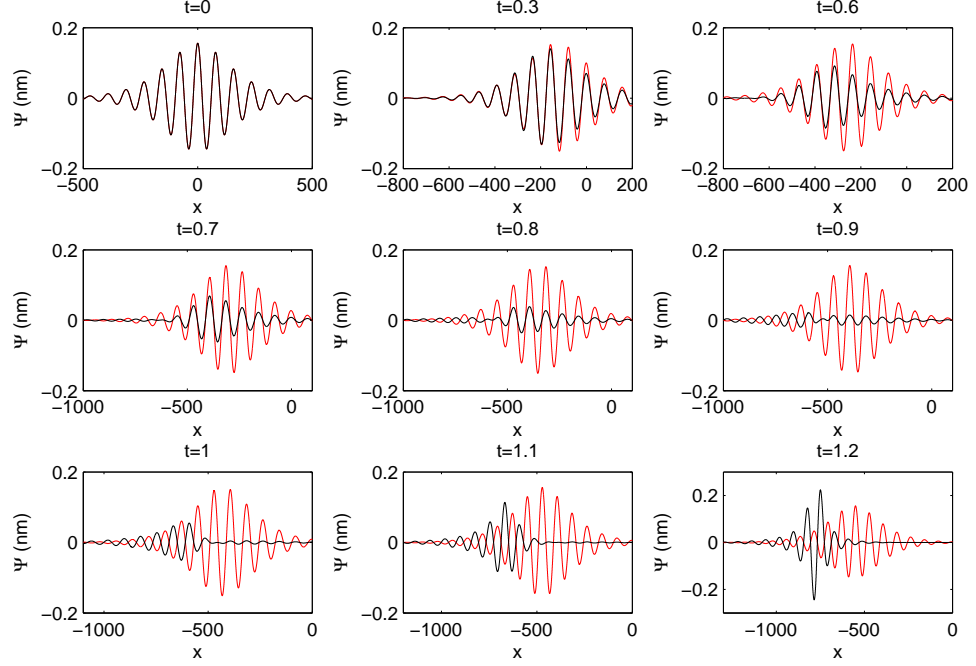
Figure 7: The DNA breathing in the model (black) and the original PB model (red) with $\gamma = 0.05$, $\bar{F} = 15e^{i\xi}$, $K = 4$ Nm, $v_e = 10^4$ m/s and $u_c = 4 \times 10^3$ m/s.

also found that the higher harmonic terms are enhanced when the periodic force is applied.

These results shows that the external force contributes constructively to accelerate the separation of double helix into single helix. More comprehensive numerical investigation of the variational equation found in this paper is still in progress.

Acknowledgments

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